

Some Representations of the Multivariate Bernoulli and Binomial Distributions

JOZEF L. TEUGELS

Katholieke Universiteit Leuven, B-3030 Heverlee, Belgium

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Multivariate but vectorized versions for Bernoulli and binomial distributions are established using the concept of Kronecker product from matrix calculus. The multivariate Bernoulli distribution entails a parameterized model, that provides an alternative to the traditional log-linear model for binary variables. © 1990 Academic Press, Inc.

1. INTRODUCTION

Assume $\{X_i, i = 1, 2, \dots, n\}$ is a sequence of Bernoulli random variables, i.e., for $i = 1, 2, \dots, n$,

$$P\{X_i = 0\} = q_i, \quad P\{X_i = 1\} = p_i,$$

where $0 < p_i = 1 - q_i < 1$. Note that $EX_i = 1 - q_i < 1$.

We look for an algebraically convenient representation for the *multivariate Bernoulli distribution*

$$p_{k_1, k_2, \dots, k_n} := P\{X_1 = k_1, X_2 = k_2, \dots, X_n = k_n\}, \quad (1.1)$$

where we assume that $k_i \in \{0, 1\}$, $i = 1, 2, \dots, n$. The representation should be amply parameterized by the n mean values $\{p_i, i = 1, 2, \dots, n\}$ and by other parameters expressing the possible dependencies among the $\{X_i, i = 1, 2, \dots, n\}$.

EXAMPLE 1.1. Let $n = 2$. Here $p_{00} = P\{X_1 = 0, X_2 = 0\}$, $p_{10} = P\{X_1 = 1, X_2 = 0\}$, $p_{01} = P\{X_1 = 0, X_2 = 1\}$, and $p_{11} = P\{X_1 = 1, X_2 = 1\}$. Furthermore $p_{00} + p_{10} + p_{01} + p_{11} = 1$ so that the distribution can be

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characterized by three parameters. However there are three "natural" parameters for $n=2$, i.e.,

$$\begin{aligned} p_1 &= EX_1 = P\{X_1 = 1\} \\ p_2 &= EX_2 = P\{X_2 = 1\} \\ \sigma_{12} &:= E(X_1 - p_1)(X_2 - p_2). \end{aligned}$$

Alternatively we can use $\mu_{12} := EX_1 X_2 = \sigma_{12} + p_1 \cdot p_2 = p_{11}$. Solving for p_{00} , p_{10} , p_{01} , and p_{11} we obtain the following two representations

$$\begin{aligned} p_{00} &= q_1 q_2 + \sigma_{12} = 1 - p_1 - p_2 + \mu_{12} \\ p_{10} &= p_1 q_2 - \sigma_{12} = p_1 - \mu_{12} \\ p_{01} &= q_1 p_2 - \sigma_{12} = p_2 - \mu_{12} \\ p_{11} &= p_1 p_2 + \sigma_{12} = \mu_{12}. \end{aligned}$$

Notice that X_1 and X_2 will be independent iff $\sigma_{12} = 0$; the first representation nicely separates the independence part from the dependency quantity σ_{12} . We can cast the representation in matrix form:

$$\begin{aligned} \begin{bmatrix} p_{00} \\ p_{10} \\ p_{01} \\ p_{11} \end{bmatrix} &= \begin{bmatrix} q_1 q_2 & -q_2 & -q_1 & 1 \\ p_1 q_2 & q_2 & -p_1 & -1 \\ q_1 p_2 & -p_2 & q_1 & -1 \\ p_1 p_2 & p_2 & p_1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ \sigma_{12} \end{bmatrix} \\ &= \begin{bmatrix} 1 & -1 & -1 & 1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ p_1 \\ p_2 \\ \mu_{12} \end{bmatrix}. \end{aligned}$$

The latter can in turn be rewritten in terms of *Kronecker products*. Put $\mathbf{p}^{(2)}$ for the vector on the left; then we have

$$\mathbf{p}^{(2)} = \begin{bmatrix} q_2 & -1 \\ p_2 & 1 \end{bmatrix} \otimes \begin{bmatrix} q_1 & -1 \\ p_1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ \sigma_{12} \end{bmatrix}$$

and

$$\mathbf{p}^{(2)} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ p_1 \\ p_2 \\ \mu_{12} \end{bmatrix}.$$

EXAMPLE 1.2. Let $n = 3$. Put

$$\mathbf{p}^{(3)} = (p_{000}, p_{100}, p_{010}, p_{110}, p_{001}, p_{101}, p_{011}, p_{111})^T$$

where $(\)^T$ stands for the transpose. We need seven parameters to characterize this distribution. On the other hand, seven natural parameters are

$$p_i = EX_i, \quad i = 1, 2, 3$$

$$\sigma_{ij} = E(X_i - p_i)(X_j - p_j), \quad (i, j) \in \{(1, 2), (1, 3), (2, 3)\},$$

$$\theta := E(X_1 - p_1)(X_2 - p_2)(X_3 - p_3).$$

In the same way as above one can find the following representation

$$p_{000} = q_1 q_2 q_3 + q_3 \sigma_{12} + q_2 \sigma_{13} + q_1 \sigma_{23} - \theta$$

$$p_{100} = p_1 q_2 q_3 - q_3 \sigma_{12} - q_2 \sigma_{13} + p_1 \sigma_{23} + \theta$$

$$p_{010} = q_1 p_2 q_3 - q_3 \sigma_{12} + p_2 \sigma_{13} - q_1 \sigma_{23} + \theta$$

$$p_{110} = p_1 p_2 q_3 + q_3 \sigma_{12} - p_2 \sigma_{13} - p_1 \sigma_{23} - \theta$$

$$p_{001} = q_1 q_2 p_3 + p_3 \sigma_{12} - q_2 \sigma_{13} - q_1 \sigma_{23} + \theta$$

$$p_{101} = p_1 q_2 p_3 - p_3 \sigma_{12} + q_2 \sigma_{13} - p_1 \sigma_{23} - \theta$$

$$p_{011} = q_1 p_2 p_3 - p_3 \sigma_{12} - p_2 \sigma_{13} + q_1 \sigma_{23} - \theta$$

$$p_{111} = p_1 p_2 p_3 + p_3 \sigma_{12} + p_2 \sigma_{13} + p_1 \sigma_{23} + \theta.$$

Again the Kronecker form can be given

$$\mathbf{p}^{(3)} = \begin{bmatrix} q_3 & -1 \\ p_3 & 1 \end{bmatrix} \otimes \begin{bmatrix} q_2 & -1 \\ p_2 & 1 \end{bmatrix} \otimes \begin{bmatrix} q_1 & -1 \\ p_1 & 1 \end{bmatrix} \cdot (1, 0, 0, \sigma_{12}, 0, \sigma_{13}, \sigma_{23}, \theta)^T.$$

The latter expression seems easily generalizable.

2. THE MULTIVARIATE BERNOULLI DISTRIBUTION

2.1. Derivation

We start by introducing a general notation for $\mathbf{p}^{(n)}$, a vector containing 2^n components. For $1 \leq k \leq 2^n$ write k in a *binary expansion*, i.e.,

$$k = 1 + \sum_{i=1}^n k_i 2^{i-1}, \quad (2.1)$$

where $k_i \in \{0, 1\}$. This expansion induces a 1-1 correspondence

$$k \leftrightarrow (k_1, k_2, \dots, k_n)$$

so that with (1.1)

$$p_k^{(n)} = p_{k_1, k_2, \dots, k_n}, \quad 1 \leq k \leq 2^n.$$

If we introduce

$$\bar{X}_i = 1 - X_i, \quad i = 1, 2, \dots, n,$$

then we can write

$$p_k^{(n)} = P \left\{ \bigcap_{i=1}^n [X_i = k_i] \right\} = E \left\{ \prod_{i=1}^n X_i^{k_i} \bar{X}_i^{1-k_i} \right\}.$$

The expression on the right can be considered as an element from a Kronecker product. In general we have the following formula for the Kronecker product of 2×1 vectors:

$$\left[\begin{bmatrix} a_n \\ b_n \end{bmatrix} \otimes \begin{bmatrix} a_{n-1} \\ b_{n-1} \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} a_1 \\ b_1 \end{bmatrix} \right]_k = \prod_{i=1}^n a_i^{1-k_i} b_i^{k_i}, \quad 1 \leq k \leq 2^n, \quad (2.2)$$

where k is given by (2.1). Putting $a_i = \bar{X}_i$ and $b_i = X_i$, we obtain the starting formula for $\mathbf{p}^{(n)}$,

$$\mathbf{p}^{(n)} = E \left[\begin{bmatrix} \bar{X}_n \\ X_n \end{bmatrix} \otimes \begin{bmatrix} \bar{X}_{n-1} \\ X_{n-1} \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} \bar{X}_1 \\ X_1 \end{bmatrix} \right]. \quad (2.3)$$

We want to express $\mathbf{p}^{(n)}$ in terms of the vector of *ordinary moments*,

$$\boldsymbol{\mu}^{(n)} = (\mu_1^{(n)}, \mu_2^{(n)}, \dots, \mu_{2^n}^{(n)})^T,$$

where

$$\mu_k^{(n)} = E \left(\prod_{i=1}^n X_i^{k_i} \right) = E \left[\begin{bmatrix} 1 \\ X_n \end{bmatrix} \otimes \begin{bmatrix} 1 \\ X_{n-1} \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} 1 \\ X_1 \end{bmatrix} \right]_k \quad (2.4)$$

and k is given by (2.1). Relation (2.4) follows from (2.2) by the choice $a_i = 1$, $b_i = X_i$.

Another representation makes use of the *central moments* expressed in the *dependency vector*

$$\boldsymbol{\sigma}^{(n)} = (\sigma_1^{(n)}, \sigma_2^{(n)}, \dots, \sigma_{2^n}^{(n)})^T,$$

where

$$\sigma_k^{(n)} = E \left(\prod_{i=1}^n (X_i - p_i)^{k_i} \right) = E \left[\begin{bmatrix} 1 \\ Y_n \end{bmatrix} \otimes \begin{bmatrix} 1 \\ Y_{n-1} \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} 1 \\ Y_1 \end{bmatrix} \right]_k$$

and $Y_i = X_i - p_i$, $i = 1, 2, \dots, n$.

Both representations are combined in our first result.

THEOREM 1. With $\mathbf{p}^{(n)}$, $\boldsymbol{\mu}^{(n)}$, and $\boldsymbol{\sigma}^{(n)}$ defined above, we have:

(i)

$$\mathbf{p}^{(n)} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}^{\otimes n} \boldsymbol{\mu}^{(n)} \quad (2.5)$$

and

$$\boldsymbol{\mu}^{(n)} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}^{\otimes n} \mathbf{p}^{(n)}; \quad (2.6)$$

(ii)

$$\mathbf{p}^{(n)} = \begin{bmatrix} q_n & -1 \\ p_n & 1 \end{bmatrix} \otimes \begin{bmatrix} q_{n-1} & -1 \\ p_{n-1} & 1 \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} q_1 & -1 \\ p_1 & 1 \end{bmatrix} \boldsymbol{\sigma}^{(n)} \quad (2.7)$$

and

$$\boldsymbol{\sigma}^{(n)} = \begin{bmatrix} 1 & 1 \\ -p_n & q_n \end{bmatrix} \otimes \begin{bmatrix} 1 & 1 \\ -p_{n-1} & q_{n-1} \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 1 & 1 \\ -p_1 & q_1 \end{bmatrix} \mathbf{p}^{(n)}. \quad (2.8)$$

Proof. (i) Note that

$$\begin{bmatrix} \bar{X}_i \\ X_i \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ X_i \end{bmatrix}, \quad i = 1, 2, \dots, n.$$

Filling this into (2.3), we have

$$\begin{aligned} \mathbf{p}^{(n)} &= E \left[\begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \right] \otimes \begin{bmatrix} 1 \\ X_n \end{bmatrix} \cdot \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \\ &\quad \otimes \begin{bmatrix} 1 \\ X_{n-1} \end{bmatrix} \cdots \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ X_1 \end{bmatrix} \end{aligned}$$

Apply the *mixed product rule* of matrix calculus [7],

$$(A \otimes B) \cdot (C \otimes D) = (A \cdot C) \otimes (B \cdot D), \quad (2.9)$$

$n-1$ times to obtain

$$\mathbf{p}^{(n)} = E \left[\begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}^{\otimes n} \begin{bmatrix} 1 \\ X_n \end{bmatrix} \otimes \begin{bmatrix} 1 \\ X_{n-1} \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 1 \\ X_1 \end{bmatrix} \right].$$

By an application of the linearity of E we find (2.5) by (2.4). The other formula derives from the rule of matrix calculus [7],

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1} \quad (2.10)$$

and easy algebra.

(ii) Clearly

$$\begin{bmatrix} 1 \\ X_i \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ p_i & 1 \end{bmatrix} \begin{bmatrix} 1 \\ Y_i \end{bmatrix}, \quad i = 1, 2, \dots, n,$$

and hence,

$$\begin{bmatrix} \bar{X}_i \\ X_i \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ X_i \end{bmatrix} = \begin{bmatrix} q_i & -1 \\ p_i & 1 \end{bmatrix} \begin{bmatrix} 1 \\ Y_i \end{bmatrix}.$$

The remaining calculations are as in case (i). ■

A slightly different proof of (ii) could be based on the following formulas, linking $\mu^{(n)}$ and $\sigma^{(n)}$:

$$\mu^{(n)} = \begin{bmatrix} 1 & 0 \\ p_n & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ p_{n-1} & 1 \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} 1 & 0 \\ p_1 & 1 \end{bmatrix} \sigma^{(n)}$$

and

$$\sigma^{(n)} = \begin{bmatrix} 1 & 0 \\ -p_n & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ -p_{n-1} & 1 \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} 1 & 0 \\ -p_1 & 1 \end{bmatrix} \mu^{(n)}.$$

For future reference we mention another property of the Kronecker product [7],

$$(A \otimes B)^T = A^T \otimes B^T. \quad (2.11)$$

The above formulas easily lead to expressions for the *marginal distributions*.

EXAMPLE 2.1. Let again $n=3$. Then the three possible marginal distributions containing two of the three r.v.'s are given by (I_m is an $m \times m$ identity matrix):

- (i) $(1, 1) \otimes I_2 \otimes I_2 \mathbf{p}^{(3)}$ for X_1 and X_2 ,
- (ii) $I_2 \otimes (1, 1) \otimes I_2 \mathbf{p}^{(3)}$ for X_1 and X_3 ,
- (iii) $I_2 \otimes I_2 \otimes (1, 1) \mathbf{p}^{(3)}$ for X_2 and X_3 .

2.2. Generating Function

We now derive a number of equivalent expressions for the (*probability*) *generating function* of the multivariate Bernoulli distribution

$$\varphi(z_1, z_2, \dots, z_n) = E(z_1^{X_1} z_2^{X_2} \dots z_n^{X_n}),$$

where z_1, z_2, \dots, z_n are n (complex) numbers.

THEOREM 2. (i) $\varphi(z_1, z_2, \dots, z_n) = \sum_{k=1}^{2^n} \omega_k(z_1, z_2, \dots, z_n) \mu_k^{(n)}$, where k is given by (2.1) and

$$\omega_k(z_1, z_2, \dots, z_n) = \prod_{i=1}^n (z_i - 1)^{k_i}, \quad 1 \leq k \leq 2^n;$$

(ii) $\varphi(z_1, z_2, \dots, z_n) = \sum_{k=1}^{2^n} \theta_k(z_1, z_2, \dots, z_n) \sigma_k^{(n)}$, where k is given by (2.1) and

$$\theta_k(z_1, z_2, \dots, z_n) = \prod_{i=1}^n (q_i + p_i z_i)^{1-k_i} (z_i - 1)^{k_i}, \quad 1 \leq k \leq 2^n.$$

Proof. By the fact that $X_i \in \{0, 1\}$ we see that

$$z_i^{X_i} = \bar{X}_i + z_i X_i = (1, z_i) \begin{pmatrix} \bar{X}_i \\ X_i \end{pmatrix}.$$

Then

$$\begin{aligned} \varphi(z_1, z_2, \dots, z_n) &= E \left(\prod_{i=1}^n (1, z_i) \cdot \begin{pmatrix} \bar{X}_i \\ X_i \end{pmatrix} \right) \\ &= E \left((1, z_n) \begin{pmatrix} \bar{X}_n \\ X_n \end{pmatrix} \otimes \dots \otimes (1, z_1) \begin{pmatrix} \bar{X}_1 \\ X_1 \end{pmatrix} \right). \end{aligned}$$

Hence by the mixed product rule and (2.3) we have

$$\varphi(z_1, z_2, \dots, z_n) = (1, z_n) \otimes \dots \otimes (1, z_1) \cdot \mathbf{p}^{(n)}.$$

(i) Use this relation together with (2.5) and the mixed product rule again to find

$$\varphi(z_1, z_2, \dots, z_n) = (1, z_n) \cdot \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} \otimes \dots \otimes (1, z_1) \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} \mu^{(n)}.$$

But

$$(1, z_i) \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} = (1, z_i - 1), \quad i = 1, 2, \dots, n$$

and so

$$\varphi(z_1, z_2, \dots, z_n) = (1, z_n - 1) \otimes \dots \otimes (1, z_1 - 1) \boldsymbol{\mu}^{(n)}.$$

To the last formula we apply the transposed version of (2.2) with $a_i = 1$, $b_i = z_i - 1$, to obtain the first formula.

(ii) The proof is entirely similar. ■

EXAMPLE 2.2. For $n = 2$ we have the formulas,

$$\varphi(z_1, z_2) = \begin{cases} p_{00} + z_1 p_{10} + z_2 p_{01} + z_1 z_2 p_{11}, \\ 1 + (z_1 - 1)p_1 + (z_2 - 1)p_2 + (z_1 - 1)(z_2 - 1)\mu_{11}, \\ (q_1 + p_1 z_1)(q_2 + p_2 z_2) + (z_1 - 1)(z_2 - 1)\sigma_{11}. \end{cases}$$

The last expression best refers to the case of eventual independence, when $\varphi(z_1, z_2) = \varphi(z_1, 1) \varphi(1, z_2)$ iff $\sigma_{11} = 0$.

2.3. Some Comments on the Multivariate Bernoulli Distribution

(i) The representation (2.5) in Theorem 1 contains $2^n - 1$ parameters since $\mu_1^{(n)} = 1$. The number of parameters in (2.7) is also $2^n - 1$; $2^n - n - 1$ are obtained in $\boldsymbol{\sigma}^{(n)}$, since $\sigma_k^{(n)} = 0$ whenever $k_1 + k_2 + \dots + k_n = 1$; the n remaining parameters are, of course, $\{p_i, 1 \leq i \leq n\}$. The representation (2.7) can be written as $\mathbf{p}^{(n)} = A_n \boldsymbol{\sigma}^{(n)}$; here $A_n \cdot \mathbf{e}_1^{(n)}$ is the representation of $\mathbf{p}^{(n)}$ under the assumption of independence of all r.v. $\{X_i, i = 1, 2, \dots, n\}$. In general the non-null components of $\boldsymbol{\sigma}^{(n)}$ express in a transparent way the $2^n - n - 1$ possible dependencies that might exist between any subset (of at least 2) of the r.v. $\{X_i, i = 1, 2, \dots, n\}$. The term dependence vector seems therefore appropriate.

(ii) In the analysis of cross-tabulated data one often uses *log-linear models*. See, for example, [3, 12]. For $n = 3$ the fully saturated model has the following log-linear representation in terms of Kronecker products; for $n = 2$, see [4];

$$\mathbf{v}^{(3)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^{\otimes 3} \boldsymbol{\lambda}^{(3)},$$

where $v_{ijk} = \log p_{ijk}$, $i, j, k \in \{0, 1\}$ and where

$$(\boldsymbol{\lambda}^{(3)})^T = (\mu, \lambda_1, \lambda_2, \lambda_{12}, \lambda_3, \lambda_{13}, 0, \varphi).$$

Compare this representation with that of Example 1.2. The number of parameters is also seven, but the direct interpretation is different.

The representation $\mathbf{p}^{(n)} = A_n \boldsymbol{\sigma}^{(n)}$ allows $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0$ without $\theta = 0$; hence there is no need for hierarchical structures like with the log-linear

representation. Also no particular problems arise when one or more of p_{ijk} happen to be zero, a situation hardly possible in the log-linear case.

Let us stress that the multivariate Bernoulli distribution only uses 0-1 variables while log-linear models have a much wider applicability.

(iii) To express the dependence between the different r.v.'s, a variety of *measures of association* can be defined. Let us restrict attention to the case $n = 3$. A tedious calculation using the notation of Example 1.2 shows that

$$p_{111} p_{001} - p_{101} p_{011} = \sigma_{12} p_3^2 - \sigma_{13} \sigma_{23} + p_3 \theta$$

$$p_{110} p_{000} - p_{100} p_{010} = \sigma_{12} q_3^2 - \sigma_{13} \sigma_{23} - q_3 \theta.$$

The quantities [3, 12]

$$\frac{p_{111} p_{001}}{p_{101} p_{011}}, \quad \frac{p_{110} p_{000}}{p_{100} p_{010}}$$

are often used to describe the interaction among X_1 , X_2 , and X_3 . From our model it seems natural to look at differences rather than at ratios. For example, X_1 and X_2 will be conditionally independent, given X_3 , iff the two ratios are one, or iff

$$\sigma_{12} p_3^2 - \sigma_{13} \sigma_{23} + p_3 \theta = 0$$

$$\sigma_{12} q_3^2 - \sigma_{13} \sigma_{23} - q_3 \theta = 0.$$

This can be rewritten in the form

$$\sigma_{12}(p_3 - q_3) + \theta = 0$$

$$\rho_{13} \cdot \rho_{23} = \rho_{12},$$

where $\rho_{ij} = \sigma_{ij} / \sqrt{p_i q_i p_j q_j}$, $i, j \in \{1, 2, 3\}$, are the *correlation coefficients*.

3. THE MULTIVARIATE BINOMIAL DISTRIBUTION

Our starting point is the multivariate Bernoulli distribution where $p_i = EX_i$ and $\sigma^{(n)}$ is the dependency vector. We take a sample of size m from (X_1, X_2, \dots, X_n) , say,

$$\{(X_{1i}, X_{2i}, \dots, X_{ni}), i = 1, 2, \dots, m\};$$

we form the multivariate sum

$$(S_{1m}, S_{2m}, \dots, S_{nm}).$$

where $S_{im} = X_{i1} + \dots + X_{im}$, $i = 1, 2, \dots, n$. We write for the joint distribution of (S_{1m}, \dots, S_{nm}) where $0 \leq r_i \leq m$, $1 \leq i \leq n$,

$$\pi_{r_1, r_2, \dots, r_n}^{(m)} = P\{S_{1m} = r_1, S_{2m} = r_2, \dots, S_{nm} = r_n\}.$$

To vectorize this n -dimensional scheme we write

$$k = 1 + \sum_{i=1}^n r_i(m+1)^{i-1}, \quad r_i \in \{0, 1, \dots, m\}.$$

Then we associate with the n -tuple (r_1, r_2, \dots, r_n) the k th element of a vector

$${}_n\mathbf{q}^{(m)} := ({}_nq_1^{(m)}, {}_nq_2^{(m)}, \dots, {}_nq_{(m+1)^2}^{(m)})^T$$

by the 1-1 correspondence,

$${}_nq_k^{(m)} := \pi_{r_1, r_2, \dots, r_n}^{(m)}, \quad 1 \leq k \leq (m+1)^n.$$

The vector ${}_n\mathbf{q}^{(m)}$ will be called the (vectorized) *multivariate binomial distribution*.

The fundamental relationship between $\pi^{(m)}$ and ${}_n\mathbf{q}^{(m)}$ is most easily seen by looking at the generating function. The proof of the following lemma can be obtained by induction.

LEMMA 3. For $m \in \{1, 2, \dots\}$,

$$\begin{aligned} \varphi^m(z_1, z_2, \dots, z_n) &= \sum_{r_1=0}^m z_1^{r_1} \sum_{r_2=0}^m z_2^{r_2} \dots \sum_{r_n=0}^m z_n^{r_n} \pi_{r_1, r_2, \dots, r_n}^{(m)} \\ &= (\mathbf{v}_n^{(m)} \otimes \mathbf{v}_{n-1}^{(m)} \otimes \dots \otimes \mathbf{v}_1^{(m)})^T {}_n\mathbf{q}^{(m)}, \end{aligned} \quad (3.1)$$

where for $i \in \{1, 2, \dots, n\}$ and $m \geq 1$, $\mathbf{v}_i^{(m)} := (1, z_i, \dots, z_i^m)^T$. Note that for any $i \in \{1, 2, \dots, n\}$,

$$(q_i + p_i z_i)(\mathbf{v}_i^{(m)})^T = (\mathbf{v}_i^{(m+1)})^T \cdot \mathcal{Q}_{i, m+1}, \quad (3.2)$$

where

$$\mathcal{Q}_{i, m+1} = \begin{vmatrix} q_i & 0 & 0 & \dots & 0 & 0 \\ p_i & q_i & 0 & \dots & 0 & 0 \\ 0 & p_i & q_i & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & p_i & q_i \\ 0 & 0 & 0 & \dots & 0 & p_i \end{vmatrix} \quad (3.3)$$

is a $(m+2) \times (m+1)$ matrix, depending solely on p_i . In a similar manner,

$$(z_i - 1)(\mathbf{v}_i^{(m)})^T = (\mathbf{v}_i^{(m+1)})^T J_{m+1}, \quad (3.4)$$

where

$$J_{m+1} = \begin{pmatrix} -1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ & \cdots & & \cdots & \cdots & \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}. \quad (3.5)$$

We now derive a vector form for ${}_n \mathbf{q}^{(m)}$.

THEOREM 4. For any $n \geq 2$ and $m \geq 1$ the multivariate binomial distribution is given by

$${}_n \mathbf{q}^{(m)} = V_m^{(n)} \cdot V_{m-1}^{(n)} \cdot \cdots \cdot V_1^{(n)},$$

where

$$V_i^{(n)} = \sum_{k=1}^{2^n} \sigma_k^{(n)} R_{n,i}^{(k)} \otimes \cdots \otimes R_{1,i}^{(k)}$$

and

$$R_{m,i}^{(k)} = \begin{cases} Q_{i,m} & \text{if } k_i = 0 \\ J_m & \text{if } k_i = 1; \end{cases}$$

the matrices $Q_{i,m}$ and J_m are given by (3.3) and (3.5), respectively.

Proof. By the independence of the elements of the sample,

$$\varphi^{m+1}(z_1, z_2, \dots, z_n) = \varphi(z_1, z_2, \dots, z_n) \varphi^m(z_1, z_2, \dots, z_n). \quad (3.6)$$

Now Theorem 2(ii) gives us a relationship allowing us to write $\varphi(z_1, \dots, z_n)$ in terms of the elements of the dependency vector $\sigma^{(n)}$. Combine (3.6) and (ii) of Theorem 2 to obtain

$$\begin{aligned} (\mathbf{v}_n^{(m+1)} \otimes \cdots \otimes \mathbf{v}_1^{(m+1)})^T {}_n \mathbf{q}^{(m+1)} &= \sum_{k=1}^{2^n} \sigma_k^{(n)} \theta_k(z_1, \dots, z_n) \\ &\quad \times (\mathbf{v}_n^{(m)} \otimes \cdots \otimes \mathbf{v}_1^{(m)})^T {}_n \mathbf{q}^{(m)}. \end{aligned} \quad (3.7)$$

Apply (2.11) and Theorem 2(ii) to write

$$\theta_k(z_1, z_2, \dots, z_n) (\mathbf{v}_n^{(m)})^T \otimes \cdots \otimes (\mathbf{v}_1^{(m)})^T = w_n \otimes w_{n-1} \otimes \cdots \otimes w_1, \quad (3.8)$$

where

$$w_i := (q_i + p_i z_i)^{1-k_i} (z_i - 1)^{k_i} (\mathbf{v}_i^{(m)})^T.$$

If $k_i = 0$, then (3.2) applies; if $k_i = 1$, (3.4) applies. By the definition of $R_{m,i}^{(k)}$ we combine both statements into the single

$$w_i = (\mathbf{v}_i^{(m+1)})^T R_{m+1,i}^{(k)}. \quad (3.9)$$

Combine (3.7)–(3.9) with the mixed product rule to find

$${}_n \mathbf{q}^{(m+1)} = \sum_{k=1}^{2^n} \sigma_k^{(n)} R_{m+1,n}^{(k)} \otimes \cdots \otimes R_{m+1,1}^{(k)} {}_n \mathbf{q}^{(m)} = V_{m+1,n}^{(n)} {}_n \mathbf{q}^{(m)}.$$

An easy induction completes the proof. ■

For the special case of the *bivariate binomial distribution* one can replace Lemma 3 by the simpler formula

$${}_2 \mathbf{q}^{(m)} = \text{vec } \pi^{(m)},$$

where $\pi^{(m)}$ is the matrix with elements $\pi_{r_1, r_2}^{(m)}$ and *vec* refers to the vec-operator introduced by Neudecker in [11] and utilized in [7, 8]. There results the expression

$$\begin{aligned} {}_2 \mathbf{q}^{(m)} &= (Q_{2,m} \otimes Q_{1,m} + \sigma J_1^{\otimes 2}) \cdots (Q_{2,2} \otimes Q_{1,2} + \sigma J_2^{\otimes 2}) \\ &\quad \times (Q_{2,1} \otimes Q_{1,1} + \sigma J_1^{\otimes 2}), \end{aligned}$$

where $Q_{i,m}$ and J_m are defined by (3.3) and (3.5), respectively.

Note that

$$\begin{aligned} Q_{2,1} \otimes Q_{1,1} + \sigma J_1^{\otimes 2} &= \begin{pmatrix} q_2 \\ p_2 \end{pmatrix} \otimes \begin{pmatrix} q_1 \\ p_1 \end{pmatrix} + \sigma \begin{pmatrix} -1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} -1 \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} q_2 & -1 \\ p_2 & 1 \end{pmatrix} \otimes \begin{pmatrix} q_1 & -1 \\ p_1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \sigma \end{pmatrix} \end{aligned}$$

by an easy calculation. For earlier attempts, see [1, 2, 5, 6, 9, 10].

4. CONCLUDING REMARKS

(i) The bivariate binomial has appeared a couple of times in the literature, mostly as a stepping stone towards a bivariate Poisson distribution. See [5, 9, 10].

(ii) The vectorization used in Section 3 is necessarily restricted to distributions with a finite number of non-zero probabilities. For the bivariate case one can still use infinite matrices like in (i) above. A bivariate version of the geometric and of the negative binomial distribution is also tractable using matrix theory. See [10]. Any further multivariate extension seems more difficult.

(iii) In [13] Wishart derives expressions for the *cumulants* of the multivariate multinomial distribution. They are obtained by expanding $\log \varphi(e^{t_1}, e^{t_2}, \dots, e^{t_n})$ with respect to increasing powers of t_i , $i = 1, 2, \dots, n$. We failed in finding a relatively easy tensor formulation of his results.

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